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High-pressure X-ray diffraction, Raman, and computational studies of MgCl2 up to 1 Mbar: Extensive pressure stability of the B-MgCl2 layered structure.

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High-pressure X-ray diffraction, Raman, and computational studies of $MgCl_2$ up to 1 Mbar: Extensive pressure stability of the β-$MgCl_2$ layered structure.

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Magnesium chloride with the rhombohedral layered $CdCl_2$-type structure (α-$MgCl_2$) has been studied using x-ray diffraction and Raman spectroscopy up to 1 Mbar (at RT). The results reveal a pressure-induced second-order phase transition to a hexagonal layered CdI_2-type structure (β-$MgCl_2$) at 0.7 GPa. This phase transition mainly affects the stacking sequence of the Cl anions, resulting to a shorter *c*-axis. An anisotropic compression along the *c*-axis was observed during initial compression. Above 10 GPa, the anisotropy is altered due to the repulsion of Cl anions between adjacent perpendicular to *c*-axis Cl-layers.

According to previous theoretical studies, a series of phase transitions towards, initially, the 3D rutile structure (with 6-fold coordinated Mg cations) at ~17 GPa and to fluorite structure (with 8-fold coordinated Mg cations) at ~70 GPa are proposed. However, according to our experimental results $MgCl_2$ remains in a 2D layered structure up to 1Mbar keeping the 6-fold coordination of Mg cations. This observation contradicts with the general structural behavior of highly compressed AB_2 compounds; we conducted *ab-initio* DFT theoretical calculations to elucidate the mechanisms that extend the remarkable structural stability of $MgCl_2$.

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